1 Test Likelihood Function

Define a simple negative log-likelihood (NLL) function that models correlations and non-parabolic behavior with a small number of parameters and that scales sensibly to large dimensions n.

For the parabolic part, use a Gaussian likelihood that is scaled to have an NLL minimum value of zero at the origin:

$$-log\mathcal{L}_0(\sigma, \rho; \vec{x}) = \frac{1}{2}\,\vec{x} \cdot M^{-1}(\sigma, \rho) \cdot \vec{x}$$

where M is the covariance for parameters having identical variances σ^2 and pair-wise correlation coefficients ρ:

$$M_{i,i} = \sigma^2 \quad , \quad M_{i,j} = \rho\sigma^2$$

with inverse

$$M^{-1}_{i,i} = \frac{1 + (n-2)\rho}{\Delta} \quad , \quad M^{-1}_{i,j} = \frac{-\rho}{\Delta} \quad , \quad \Delta \equiv (1-\rho)(1+(n-1)\rho)\sigma^2 \; .$$

Note that the requirement of a non-zero determinant

$$\det M = (1 + (n-1)\rho)(1-\rho)^{n-1}\sigma^{2n}$$

adds an additional restriction $\rho \neq -1/(n-1)$ to the usual $\sigma > 0$ and $|\rho| < 1$. The parabolic partial derivatives are:

$$G_{i,0}(\sigma, \rho; \vec{x}) \equiv \frac{\partial}{\partial x_i}\Big(-\log\mathcal{L}_0(\sigma, \rho; \vec{x})\Big) = \frac{2x_i}{(1-\rho)\sigma^2} - 2\rho\frac{\Sigma_x}{\Delta}$$

with

$$\Sigma_x \equiv \sum_i x_i \; .$$

Add non-parabolic behavior via a single parameter α using the coordinate transformation:

$$y_i(\alpha; \vec{x}) = x_i - \alpha(|\vec{x}|^2 - x_i^2)$$

to obtain a non-parabolic NLL that also has a minimum value of zero at the origin:

$$-\log\mathcal{L}(\sigma, \rho, \alpha; \vec{x}) = -\log\mathcal{L}_0(\sigma, \rho; \vec{y}(\vec{x})) \; .$$

The non-parabolic partial derivatives are

$$G_i(\sigma,\rho,\alpha;\vec{x}) \equiv \frac{\partial}{\partial x_i}\Big(-\log\mathcal{L}(\sigma,\rho,\alpha;\vec{x})\Big) = \sum_j G_{j,0}(\sigma,\rho;\vec{x})\cdot\frac{\partial}{\partial x_i}y_j(\alpha;\vec{x})$$

which simplifies to

$$G_i(\sigma,\rho,\alpha;\vec{x}) = \frac{2y_i(1+2\alpha x_i)}{(1-\rho)\sigma^2} - 2(\rho+2\alpha x_i)\frac{\Sigma_y}{\Delta}$$

using

$$\frac{\partial}{\partial x_i}y_j(\alpha;\vec{x}) = \delta_{ij} - 2\alpha x_i(1-\delta_{ij})\ .$$

Figures 1 and 2 demonstrate the effects of ρ and α on this test NLL function in low dimensions, and Figure 3 shows that the essential features are preserved in high dimensions.

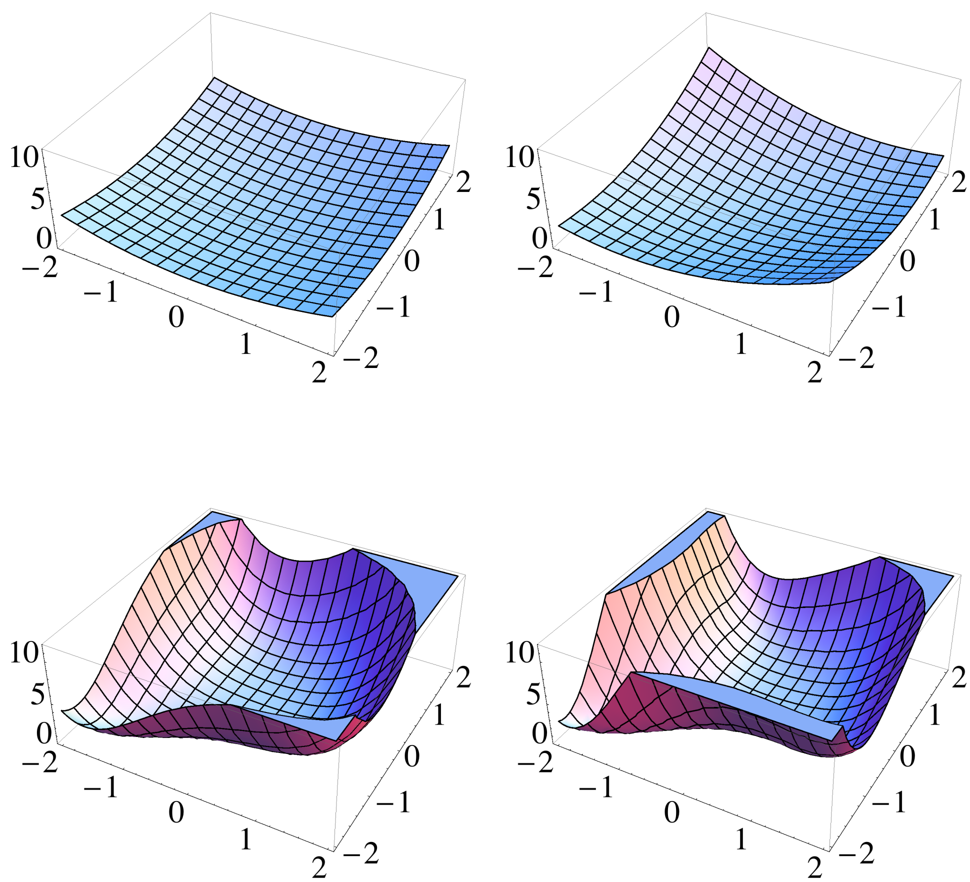

Figure 1: Two-parameter $\sigma = 1$ test NLL functions with: $\rho = \alpha = 0$ (top-left), $\rho = 0.5$ (top-right), $\alpha = -1$ (bottom-left), $\rho = 0.5$ and $\alpha = -1$ (bottom-right). All plots have the same vertical scale.

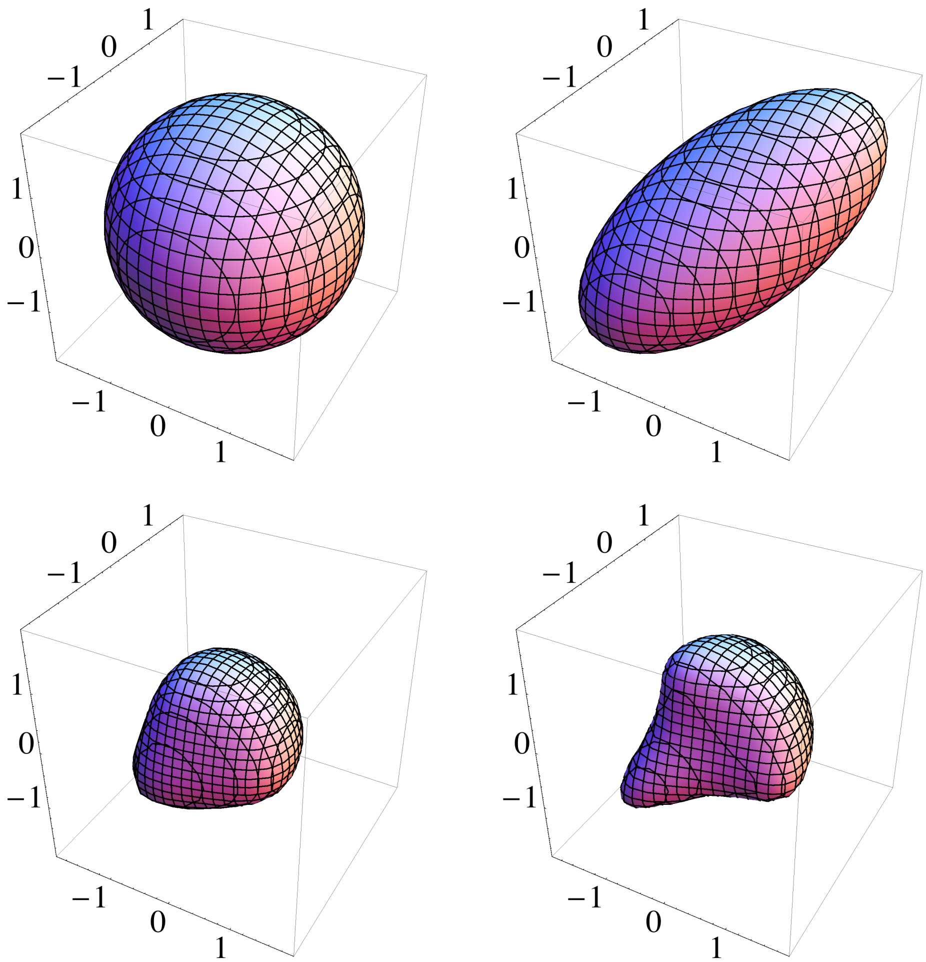

Figure 2: Three-parameter $\sigma = 1$ test NLL functions with: $\rho = \alpha = 0$ (top-left), $\rho = 0.5$ (top-right), $\alpha = -1$ (bottom-left), $\rho = 0.5$ and $\alpha = -1$ (bottom-right). Plots show contours of NLL = 1.75, which represents the 3-parameter 68% confidence-level.

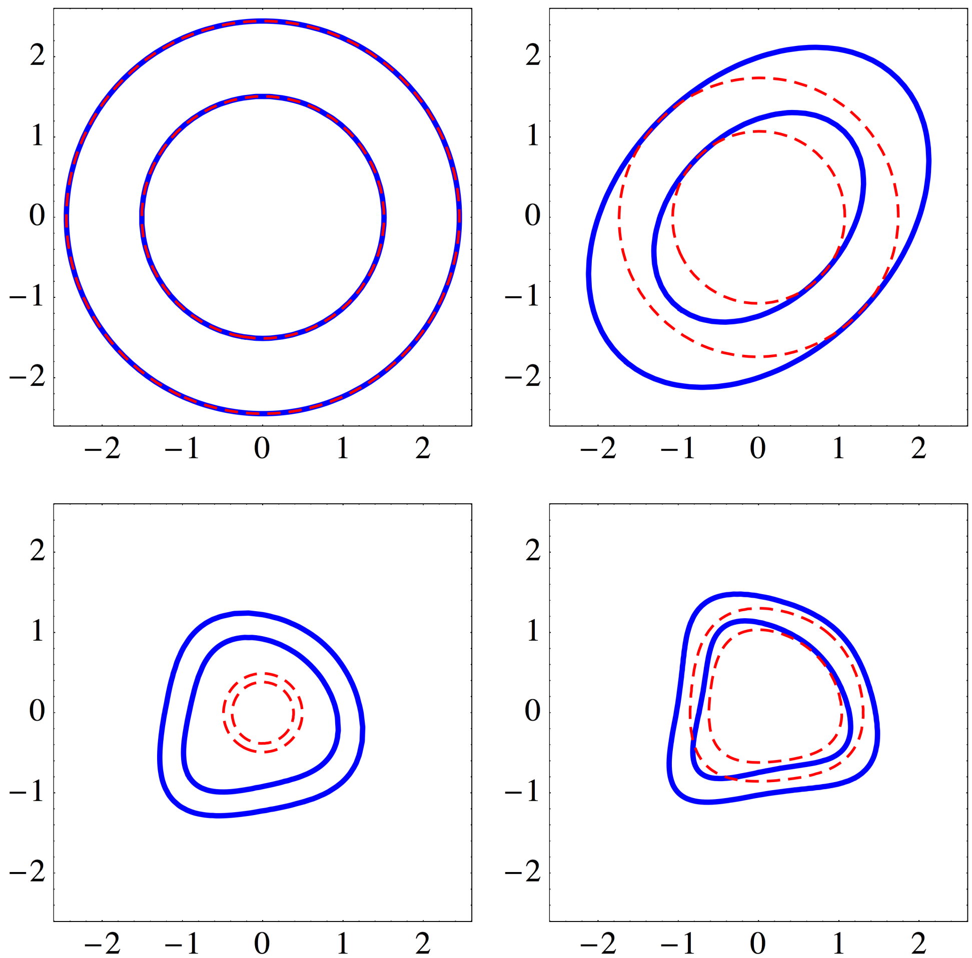

Figure 3: Three-parameter (solid blue) and 100-parameter (dashed red) $\sigma = 1$ test NLL functions with: $\rho = \alpha = 0$ (top-left), $\rho = 0.5$ (top-right), $\alpha = -1$ (bottom-left), $\rho = 0.5$ and $\alpha = -1$ (bottom-right). Plots show contours of NLL = 1.44 and 3.00, which represent the 2-parameter 68% and 95% confidence-levels, respectively.